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ENCODING THE DIHEDRAL ANGLE OF AMINO ACID IN A PROTEIN

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ABSTRACT

Proteins play an important role in cell functions. Protein structures are useful for determining its functions. Dihedral angle places an important role in determining the structure of proteins. The aim of encoding the angle of dihedral or torsion angle is done with respect to the plane of two angles. This paper explains encoding the dihedral angle of amino acids in a protein by applying the mathematical representation of determining dihedral or torsion angle with respect to the plane of two angles. By calculating the cross product and dot product of two vectors of amino acid the dihedral angle are determined.

KEYWORDS: Protein Structures, Dihedral angles, Torsion Angles & Plane of Angles, PDB

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INTRODUCTION

"A dihedral angle is defined as the angle between two intersecting planes. In Proteins, the dihedral angles are formed between the planes of two sets of three backbone atoms which can ψ, ϕ or χ^1, χ^2, χ^3 etc." The dihedral angle is used to represent the accurate conformation of protein structures along with the force field. The ψ and φ angles contribute to predicting the structure of protein. [1] Dihedral angles are mainly useful in predicting the mimetic of proteins in drug discovery. [2]

METHOD

To encode the dihedral angle of a protein, it's important to represent the protein in a proper manner. The representation of amino acids is extracted from a PDB (Protein Data Bank) data file. Figure 1 shows PDB file which contains the information with PDB number, Protein name, Residue Number, X, Y and Z co-ordinates in space.

Atom	PDB No	Protein		Residue No	X	Y	Z	Atom
ATOM	1	N	HIS A	1	49.668	24.248	10.436	N
ATOM	2	CA	HIS A	1	50.197	25.578	10.784	C
ATOM	3	C	HIS A	1	49.169	26.701	10.917	C
ATOM	4	O	HIS A	1	48.241	26.524	11.749	O
ATOM	5	CB	HIS A	1	51.312	26.048	9.843	C
ATOM	6	CG	HIS A	1	50.958	26.068	8.340	C

Figure 1: PDB - File Information of Amino Acids with Each Atom

These PDB files do not contain the Hydrogen information; hence Hydrogen is added to the representation after accessing each residue. After Hydrogen is added, each atom is given an Atom Number and stored in a matrix along with its co-ordinates information. Figure 2 gives the representation of 3 amino acids after adding Hydrogen atom. [3]

Three Amino Acids HIS, SER, GLN are taken and represented as illustrated in the Figure 2. Starting from the first Atom Nitrogen (N) which is assigned 0, Cα assigned atom number 1, etc. All the backbone of an AA's are assigned the atom number, and then followed by the side chain molecules; last, the Hydrogen atoms are assigned Atom numbers. Similarly, all AA's are assigned the atom number.

- **Representation of Dihedral Angles**

After all AA's are represented with atom number, a need to represent the dihedral angle is done. Figure 3 shows the representation of dihedral angle. By considering the dihedral angle to be encoded to be present in the i^{th} AA, its previous AA is taken as i-1 and next AA is taken as i+1. Cαi has ϕ and ψ angles respectively. The plane of two angles are given as C_{i-1} — N_i — $C_{\alpha i}$ and N_i — $C_{\alpha i}$— C_i.

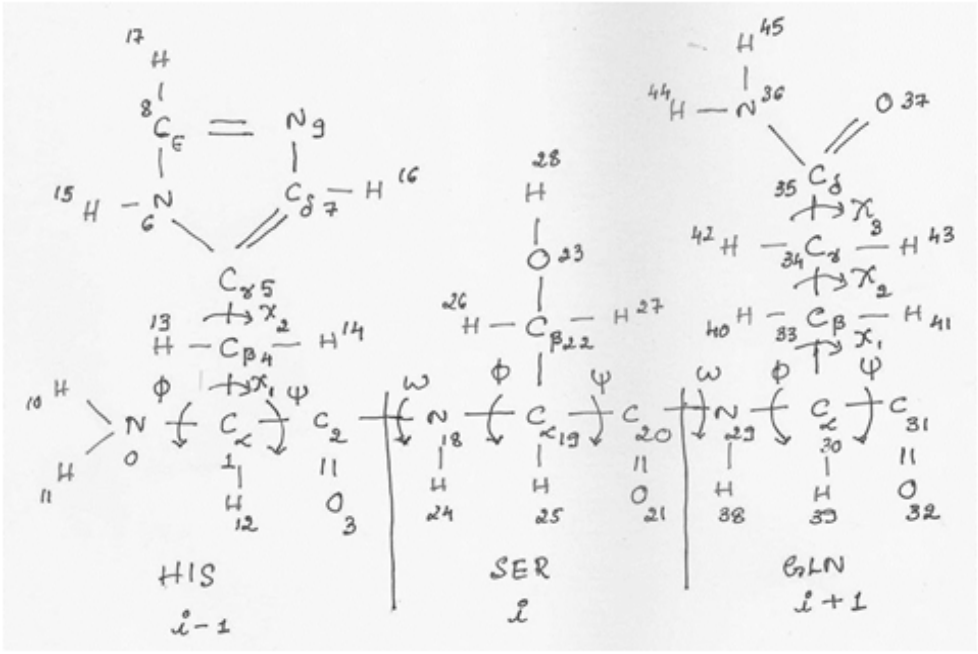

Figure 2: Representation of 3 Amino Acids of a Protein

ϕ: C_{i-1} — N_i — $C\alpha_i$ — C_i
Ψ: N_i — $C\alpha_i$— C_i— N_{i+1}
χ_1: N_i — $C\alpha_i$— $C\beta_i$— $C\gamma_i$

Figure 3: Representation of Dihedral Angle

- **Encoding the Dihedral Angles**

To encode the dihedral angle, select the atom number as illustrated in Figure 4. In the following case by considering the Figure 2, atom number 19 is selected and corresponding co-ordinates from the PDB file are accessed as shown in Table 1.

ϕ: C_2 — N_{18} — $C\alpha_{19}$ — C_{20} (ϕ over N_{18}—$C\alpha_{19}$, Ψ over $C\alpha_{19}$—C_{20})

Figure 4: To Encode the Dihedral Angle of Cα19 Atom

Table 1: Co-Ordinates of 4 Atoms from PDB

Atom	Amino Acid	X	Y	Z
C_2	HISTIDINE	49.169	26.701	10.917
N_{18}	SERINE	49.788	27.850	10.784
$C_{\alpha 19}$	SERINE	49.138	29.147	10.620
C_{20}	SERINE	47.718	29.251	10.110

- **Mathematical Representation of Dihedral Angle**

Dihedral angles are the angles between two planes as shown in Figure 5, mathematically it can be calculated using the Cross product and Dot product of Vectors. [4]

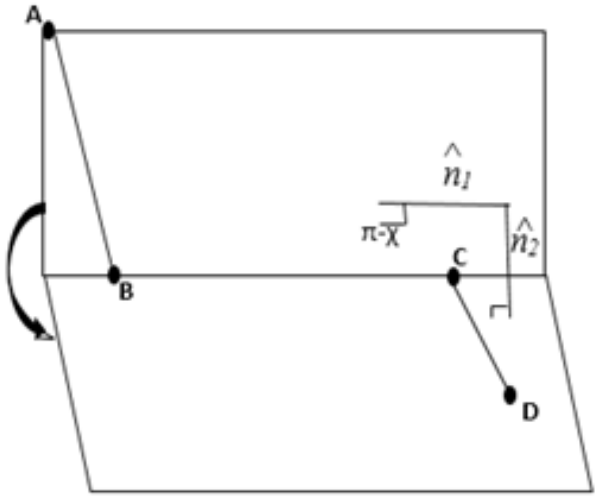

Figure 5: Representation of Dihedral Angles between Two Planes

The Eq. used to calculate the vector $\widehat{n_1}$and $\widehat{n_2}$is given below.

$$\widehat{n_1} = \frac{\overrightarrow{AB} * \overrightarrow{BC}}{|\overrightarrow{AB}||\overrightarrow{BC}|} \quad (1)$$

$$\widehat{n_2} = \frac{\overrightarrow{BC} * \overrightarrow{CD}}{|\overrightarrow{BC}||\overrightarrow{CD}|} \quad (2)$$

Eq. (1) and (2) represents the vector AB and BC and the magnitude of vector AB and BC respectively.

$$\cos(\pi - \chi) = \widehat{n_1} \cdot \widehat{n_2} \quad (3)$$

$$\cos \chi = -\widehat{n_1} \cdot \widehat{n_2} \quad (4)$$

The dihedral angles of the atom number 19 in Figure 4 can be represented using the two planes as Plane 1 with C2 - N18 – Cα19 and Plane 2 as N18 – Cα19- C20. Using the Eq. (1) and Eq. (2), the dihedral angle can be calculated as shown in the Eq. (5). The calculation of vector and the distance is shown in Table 2 and illustrated in Figure 6.

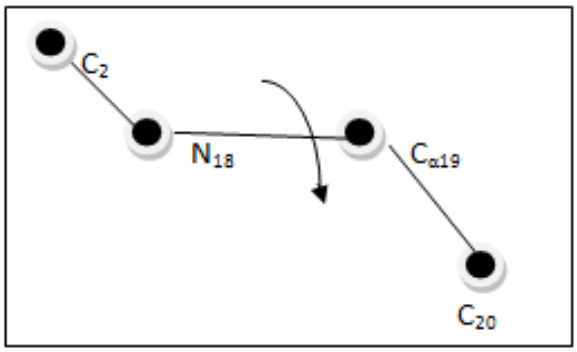

Figure 6: Representing Dihedral Angle Cα for Amino Acid SERINE in the Given Protein

- **Dihedral Angle Calculation**

The Eq. 1 and Eq. 2 to fit the amino acid is represented in Eq. 5 and Eq. 6 respectively.

$$n_1 = \frac{\overrightarrow{C_2N_{18}} * \overrightarrow{C\alpha_{19}N_{18}}}{|\overrightarrow{C_2N_{18}}|\ |\overrightarrow{C\alpha_{19}N_{18}}|} \quad (5)$$

$$n_2 = \frac{\overrightarrow{C\alpha_{19}N_{18}} * \overrightarrow{C_{20}C\alpha_{19}}}{|\overrightarrow{C\alpha_{19}N_{18}}|\ |\overrightarrow{C_{20}C\alpha_{19}}|} \quad (6)$$

Calculating the X, Y, Z and Distance is illustrated below, for the vector, and the Eq. are as follows.

The corresponding values after calculation are given in Table 2.

$$X = C\alpha_{19}X - N_{18}X \quad (7)$$

$$Y = C\alpha_{19}Y - N_{18}Y \quad (8)$$

$$Z = C\alpha_{19}Z - N_{18}Z \quad (9)$$

Distance,$|\overrightarrow{C_{\alpha19}N_{18}}|$ is calculated as shown in the Eq. 10

$$\sqrt{|\overrightarrow{C_{\alpha19}N_{18}}|X * |\overrightarrow{C_{\alpha19}N_{18}}|X + |\overrightarrow{C_{\alpha19}N_{18}}|Y * |\overrightarrow{C_{\alpha19}N_{18}}|Y + |\overrightarrow{C_{\alpha19}N_{18}}|Z * |\overrightarrow{C_{\alpha19}N_{18}}|Z} \quad (10)$$

Table 2: Calculation of Vectors and its Distances

Vector	X	Y	Z	Distance
$\overrightarrow{C_{\alpha19}N_{18}}$	-0.650	1.297	-0.164	1.460
$\overrightarrow{C_2N_{18}}$	-0.619	-1.149	0.133	1.311
$\overrightarrow{C_{20}C_{\alpha19}}$	-1.425	0.104	-0.51	1.317
$\overrightarrow{C_{\alpha19}N_{18}} * \overrightarrow{C_2N_{18}}$	-2.040	-1.009	0.101	2.279
$\overrightarrow{C_{\alpha19}N_{18}} * \overrightarrow{C_2N_{18}} * \overrightarrow{C_{\alpha19}N_{18}}$	-0.015	0.187	1.549	1.561

- **Calculating Cross Product and Dot Product of Dihedral Angles**

The Cross Product of$\overrightarrow{C_{\alpha19}N_{18}} * \overrightarrow{C_2N_{18}}$ is calculated using the equation as follows and the result is placed in Table 2.

$$X = (\overrightarrow{C_{\alpha19}N_{18}}\,y * \overrightarrow{C_2N_{18}}\,z) - (\overrightarrow{C_{\alpha19}N_{18}}\,z * \overrightarrow{C_2N_{18}}\,y) \quad (11)$$

$$Y = \left(\overrightarrow{C_{\alpha 19}N_{18}}\, z * \ \overrightarrow{C_2N_{18}}\, x\right) - \ (\overrightarrow{C_{\alpha 19}N_{18}}\, x * \ \overrightarrow{C_2N_{18}}\, z) \tag{12}$$

$$Z = \left(\overrightarrow{C_{\alpha 19}N_{18}}\, x * \ \overrightarrow{C_2N_{18}}\, y\right) - \ (\overrightarrow{C_{\alpha 19}N_{18}}\, y * \ \overrightarrow{C_2N_{18}}\, x) \tag{13}$$

The Dot Product for $\widehat{n_1}$ and $\widehat{n_2}$ is calculated using the Eq.5 and Eq. 6 is applied for the amino acid atoms as follows.

$$\widehat{n1} = \frac{\overrightarrow{C_{20}C_{\alpha 19}}.\left(\overrightarrow{C_{\alpha 19}N_{18}} * \overrightarrow{C_2N_{18}}\right) * \overrightarrow{C_{\alpha 19}N_{18}}}{||\overrightarrow{C_{\alpha 19}N_{18}} * \overrightarrow{C_2N_{18}}|.|\overrightarrow{C_{\alpha 19}N_{18}}||} \tag{14}$$

$$\widehat{n2} = \frac{\overrightarrow{C_{20}C_{\alpha 19}}.\left(\overrightarrow{C_{\alpha 19}N_{18}} * \overrightarrow{C_2N_{18}}\right)}{||\overrightarrow{C_{\alpha 19}N_{18}}|.|\overrightarrow{C_2N_{18}}||} \tag{15}$$

Finally Dihedral angle ψ is calculated by

$$Cos\,\psi = \frac{\sqrt{(\widehat{n1} * \widehat{n1})}}{\sqrt{((\widehat{n2}) * (\widehat{n2}))} + (\widehat{n2}) * (\widehat{n2})} \tag{16}$$

The Dihedral angle ψ in the Eq. 16 can be rewritten as

$$\psi = \ Cos - 1\frac{\sqrt{(\widehat{n1} * \widehat{n1})}}{\sqrt{((\widehat{n2}) * (\widehat{n2}))} + (\widehat{n2}) * (\widehat{n2})} \tag{17}$$

$$\psi \ = \frac{\psi * 180}{\pi} \tag{18}$$

"The dihedral angle determines the conformations around bonds which are rotating. The change in the dihedral angle is possible with only the distance between the 1st and 4th atoms of the amino acids; the other 2 atoms would contribute only for chemical bond lengths and bond angles. Its value range from -180 to +180 degrees. The dihedral angle is considered to be +ve if a clockwise rotation is performed with the molecule and it will be -ve when an anti-clockwise rotation is performed with the molecule in its plane." [5,6, 7].

$$\text{If } (\widehat{n1} < 0), \psi \ = \ 180 - \psi \text{ else } \psi \ = \ -\psi \tag{19}$$

RESULTS AND DISCUSSIONS

The dihedral angle for $\overrightarrow{C_{\alpha 19}N_{18}}$ is calculated by accepting X of $C_{\alpha 19}$ as 49.138 and N_{18} of Eq. 7, X as 49.788, resulting with -0.65, the same is displayed in the Table 2. Similarly same value of X, Eq. 8, Y and Eq. 9, Z is calculated. The distance Eq. 10, $|\overrightarrow{C_{\alpha 19}N_{18}}|$ = 1.460. The cross product of $\overrightarrow{C_{\alpha 19}N_{18}}$ * $\overrightarrow{C_2N_{18}}$ is calculated by accepting the values from Table 2 and Eq. 11, X is calculated as (1.297 * 0.133) – (-0.164 * -1.149) resulting with -2.040. Similarly same value of X, Eq. 12, Y and Eq. 13, Z is calculated. The dot product Eq. 14, $\widehat{n1}$is calculated by accepting the values of X, Y and Z as {(-1.425 * -0.015) + (0.104 * 0.187) + (-0.51 * 1.549)} / (1.561), resulting with the value 1.3156. Similarly, Eq. 15,$\widehat{n2}$is calculated resulting with value -0.508. Finally Eq. 16, cos ψ = 0.9327 and Eq. 17 ψ is the cos-1 with value 0.3689. This Eq. 18, ψ is multiplied by 180 and divided by π. Thus the Eq. 19, ψ = 21.13. Since $\widehat{n1}$>0 the ψ = -21.13.

CONCLUSIONS

The dihedral angle 'ψ' of an amino acid is calculated, which can be the input for rotating the dihedral angle with respect to the bond length of atoms 'l', rotation angle 'Θ' and the dihedral angle 'ψ'. These 3 values can be used for rotation of dihedral angle to predict the structure of a protein.

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